Distortion blockade in classical nano-electromechanical resonator

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We consider a single electron transistor where the central island can oscillate. It has been shown that for weak coupling of the elastic and electric degrees of freedom the position of the island fluctuates with a small variation of the current through the device. In this paper we consider the strong coupling limit. We show that the system undergoes a static mechanical instability that is responsible for the opening of a gap in the current voltage characteristics even at the degeneracy point. We provide an analytical description of the transition point. We also discuss how the mechanical nature of the suppression of the current can be probed experimentally by a slow modulation of the gate voltage.

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Nanoelectromechanics constitutes a rapidly developing and promising field of mesoscopic physics [1, 2, 3]. A particularly important and investigated device is the single electron transistor with mobile parts [4, 5, 6]. Due to the Coulomb blockade the interplay between the electrical and mechanical degrees of freedom influences the current in a sizable way. When the oscillation amplitude is sufficiently large with respect to the tunnelling length, the modulation of the tunnelling rates leads to the shuttle phenomena, where the oscillations becomes synchronized with the electron tunnelling [7, 8, 9, 10]. If the oscillation does not modify the distance between source and drain, it may nevertheless induce a modulation of the tunnelling rates through the variation of the electric potential energy in space [11, 12, 13, 14, 15]. Typically this effect is due to the position dependence of the gate capacitance. If the Coulomb force generated by the variation of the number of electrons by one is F, the distance of the two equilibrium positions of the island will be $X_o = F/k$ where k is the effective elastic constant of the island. The corresponding variation of the elastic energy is $E_E = F^2/k$. For source-drain bias voltages V of the order of E_E/e (with e the electron charge), the interplay between the electrical and mechanical degrees of freedom becomes important. Typically E_E is very small, but within the range of observation. For a nanotube of 500 nm length, 1 nm radius, suspended at 100 nm from a gate E_E is of the order of 100 μeV. Previous analytic work concentrate on the case $eV \gg E_E$ [12, 16]. Very recently the current for $eV \geq E_E$ at the degeneracy point has been considered numerically [15]. In this paper we present an analytic theory that gives a good description of the whole region $eV \geq E_E$ and arbitrary gate voltage. We find that sweeping the gate voltage for $eV > E_E$ the current jumps from 0 in the blocked regions to a finite value in the conducting regions. We also discuss the behavior of the system for $eV < E_E$. We argue how a static mechanical instability blocks the current for any value of the gate voltage.

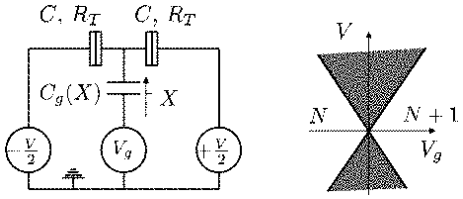

FIG. 1: Left panel: Circuit diagram for the single electron transistor with an oscillating central island. The variable X parameterizes an effective position. Right panel: conducting regions shaded in the V_g-V near a degeneracy point between N and $N+1$ electrons.

Let us consider a single electron transistor with a mobile central island (see Fig. 1). The model has been discussed in details in previous works (see for instance Refs. [12, 13, 14, 15]), we discuss the simplest configuration of symmetric capacitances, resistances, and bias at zero temperature. (Strictly speaking we assume $E_E \gg k_B T \gg \hbar\omega$.) For small oscillations gate capacitance varies linearly in the displacement of the island X. Charge transport can be described as usual by a master equation where the rates are modulated by the position of the island. For positive source drain voltage ($V > 0$), and the gate voltage V_g tuned close the degeneracy point between N and $N+1$ electrons on the island, the non vanishing rates read:

$$\Gamma_{L,R} = f(eV/2 \pm \beta_g(0) eV_g \mp (2N+1)E_C(0) \mp FX)\,, \quad (1)$$

where Γ_L and Γ_R are the rates for transfer of electrons from the left lead to the island and from the island to the right lead, respectively, R_T is the tunnelling resistance of the left and right contacts, $E_C(X) = e^2/2C_\Sigma$ is the Coulomb energy of the device as a function of the position of the island X, C and $C_g(X)$ are the junction and gate capacitances, respectively, $C_\Sigma(X) = 2C + C_g(X)$, $f(E) = E/(e^2 R_T)$ for $E > 0$ and 0 for $E < 0$, and finally $\beta_g(X) = C_g(X)/C_\Sigma(X)$. Choosing $X = 0$ as the equilibrium position for the island with N electrons, the force

acting on the island when an additional electron is added is then $F = -(2N+1)E_C[1+2C/C_g(0)]C_\Sigma^{-1}dC_g(X)/dX$, where we set $eV_g = (2N+1)E_C/\beta_g$, since we will consider small variation of V_g around this value. The motion of the island is described by the Newton equation:

$$m\ddot{X}(t) = -kX(t) - Fn(t) \tag{2}$$

where $n(t)$ fluctuates stochastically between 0 and 1 according to the rates given in Eq. (1), m is the effective mass of the island. It has been shown that the coupling to the electronic degrees of freedom introduces an intrinsic damping coefficient [12]. We thus do not introduce an extrinsic dissipation into Eq. (2), assuming that the intrinsic dissipation is dominant. It is convenient to introduce reduced variables: $x(\tau) = X/X_o$, $u = \dot{X}/(\omega_o X_o)$, $v = eV/E_E$, $v_g = (\beta_g eV_g - (2N+1)E_C)/E_E$, $\tau = \omega_o t$, $\Gamma_o = E_E/(e^2 R_T \omega_o)$, with $\omega_o^2 = k/m$. For fixed x the stationary current is given by the usual expression

$$\frac{I}{R_T V} = \frac{e}{R_T V}\frac{\Gamma_L\Gamma_R}{(\Gamma_L+\Gamma_R)} = \frac{v^2/4 - (v_g - x)^2}{v^2} \quad . \tag{3}$$

In the plane v-v_g it leads to the Coulomb diamond structure of the current, as shown in Fig. 1, with the degeneracy point sitting at $v_g = 0$ for $x = 0$.

The effect of the oscillation of the central island on the current can be studied analytically far from the boundaries of the conducting regions [12]. In that limit it has been shown that the probability distribution of x and u becomes gaussian with a width controlled by the voltage bias v, and the variation of the current due to the mechanical coupling is always a small part of the unperturbed value. In this paper we will focus on the regions near the degeneracy point and near the two lines of transition from the conducting to the non conducting region (see Fig. 1 right panel). We assume that $\Gamma_o \gg 1$ so that the problem can be tackled by exploiting the separation of time scales between the slow mechanical oscillations and the frequent electronic hopping.

We begin with a very simple description of the stochastic force by substituting into Eq. (2) the average occupation number: $n(t) \to \bar{n}(x)$, where:

$$\bar{n}(x) = \frac{v/2 + v_g - x}{v}\,, \quad \text{for } |v_g - x| < v/2\,, \tag{4}$$

$\bar{n}(x) = 0$ for $v_g - x < -v/2$, and $\bar{n}(x) = 1$ for $v_g - x > v/2$. This induces an average force on the island that depends on the occupation of the island itself. It is convenient to introduce an effective potential to describe this force (in units of E_C):

$$U_{eff}(x) = \int_{x_m}^{x} [x + \bar{n}(x)]dx \tag{5}$$

where $x_m = (v/2 + v_g)/(1 - v)$. The form of $\bar{n}(x)$ given above implies that d^2U_{eff}/dx^2 equals $(1 - 1/v)$ for $|v_g - x| < v/2$ and 1 otherwise. For $v > 1$ the potential has thus a single minimum at x_m with $-1 \le x_m \le 0$ and (by construction) $U_{eff}(x_m) = 0$. For $0 < v < 1$ instead two minima may be present, depending on the value of v_g. The evolution of the potential as a function of v is shown in Fig. 2 for $v_g = -1/2$. At $v = 1$ the potential becomes flat and for $v < 1$ it develops two side minima.

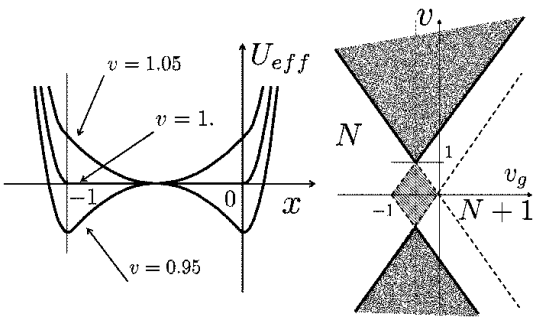

FIG. 2: Left panel: Effective potential U_{eff} for $v_g = -1/2$ and $v = 1.05$, 1, and 0.95. Right panel: Shape of the conducting regions (grey) in the plane v_g-v when the displacement of the mobile part is taken into account. The small dashed diamond indicates the mechanically bistable region.

The form of the effective potential has important consequences on the current flowing through the device. Within this simple approximation the average position x is determined by the minimum of the potential. The current is then given by Eq. (3) with $x = x_m$. Note that $x_m \le 0$, this implies that the displacement increases the gate voltage seen by electrons [cf. Eq. (1)]. Thus if for $v > 1$ we sweep v_g from negative to positive values, $\bar{n} = 0$ for $v_g < -v/2$, $\bar{n}$ then starts to increase linearly from 0 to 1. Due to the displacement of the average position $\bar{n}$ equals 1/2 (degeneracy point) at $v_g = -1/2$ instead of $v_g = 0$. For the same reason it becomes 1 at $v_g = v/2 - 1$ instead of $v_g = v/2$. The shape of the conducting region changes thus slightly for $v \gg 1$, as shown in Fig. 2. But for $v \le 1$ the consequence is more dramatic. The evolution in v_g is no more smooth, due to the presence of two minima, the system is hysteretic and the stable position and occupation jump from $x_m = -1$ and $\bar{n} = 0$ to $x_m = 0$ and $\bar{n} = 1$, or viceversa. The current is thus always blocked for $v < 1$. As shown in Fig. 2 right panel, a gap appears in the v_g-v plane at the degeneracy point. This effect can be regarded as the classical counterpart of the Frank-Condon effect in the quantum limit that has been shown to lead to a current suppression in molecular devices [17, 18, 19, 20]. The fact that this phenomenon exists also in the classical limit, makes it probably more easy to be observed in finite temperature device. Moreover, the simplicity of the classical description affords an analytical solution and the the possibility of treating more complex situation, as the non stationary evolution discussed in the following.

Let us now discuss the behavior of the system in the

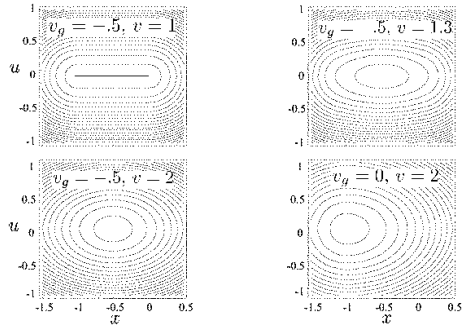

FIG. 3: Lines of equal energy and thus of equal probability $\mathcal{Q}$ in the x-u plane for the values of v and v_g indicated.

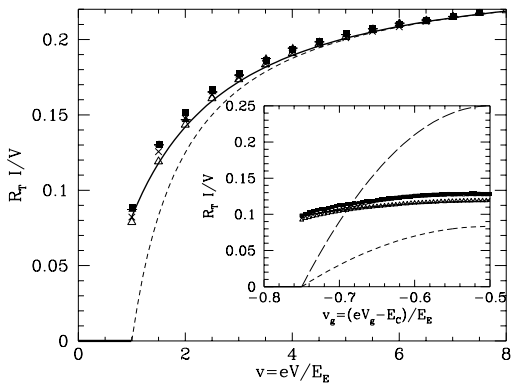

FIG. 4: Current as a function of v at $v_g = -1/2$ from the analytical calculation (full line), the weak coupling theory (dashed line) and the Monte Carlo simulation (points). The values of Γ_o are 10 (square), 1 (triangle), 0.1 (cross) and 0.01 (full square). In the inset: current as a function of v_g for $v = 1.5$. The long dashed line is Eq. (3) for $x = x_m$.

conducting region ($v > 1$). The dependence of the current and the probability distribution for x along the degeneracy line ($v_g = -1/2$, and $v > 1$) have been considered very recently in Ref. [15] numerically. We present here an analytical theory that gives a good description of the current in the whole conducting region, including near the boundaries and at the apex. For $\Gamma_o \gg 1$, the electrons have the time to hop in and out of the grain many times before it can move of a sizable distance. One can then write a Fokker-Plank equation for the probability $\mathcal{Q}(x,u)$ [13]:

$$\frac{\partial \mathcal{Q}}{\partial t} = -\frac{\partial}{\partial u}[F_e(x) - \eta_i(x)u]\mathcal{Q} - \frac{\partial}{\partial x}u\mathcal{Q} + \frac{1}{2}\frac{\partial}{\partial u^2}S(x)\mathcal{Q} \quad (6)$$

where $F_e(x) = -dU_{eff}/dx$, and $\eta_i(x) = (\partial\bar{n}/\partial v_g)/v\Gamma_o$ is the intrinsic damping [12, 14]. The non vanishing second moment is $S(x) = \int d\tau \,\langle \delta n(\tau)\delta n(\tau)\rangle = 2\bar{n}(x)(1 - \bar{n}(x))/\Gamma_o v$. It is convenient to simplify further the equation by exploiting the fact that the fluctuating and dissipative part is small for $\Gamma_o \gg 1$. The distribution function is thus a function of the effective energy:

$$E_e(x,u) = U_{eff}(x) + u^2/2\,. \quad (7)$$

From Eq. (6) we can derive an equation for $\mathcal{P}(E) \equiv \int dxdu\mathcal{Q}(x,u)\delta(E - E_e(x,u))$:

$$\frac{\partial \mathcal{P}}{\partial t} = \frac{\partial}{\partial E}\left[-\alpha(E)\mathcal{P}(E) + \frac{\partial}{\partial E}\,(\beta(E)\mathcal{P}(E))\right] \quad (8)$$

with $\alpha(E) = \left\langle S(x)/2 - \eta_i(x)u^2\right\rangle_E$ and $\beta(E) = \left\langle S(x)u^2\right\rangle_E/2$, where the averages are taken on the trajectories in the x-u plane at fixed energy E. These trajectories are shown for some values of v and v_g in Fig. 3. Near the apex and the borders the shape is quite different from an ellipse, which is the harmonic oscillator trajectory.

The stationary solution of Eq. (8) is

$$\mathcal{P}(E) = \mathcal{N}\exp\left\{\int^E dE'\alpha(E')/\beta(E')\right\}/\beta(E) \quad (9)$$

where $\mathcal{N}$ is a normalization constant. Once $\mathcal{P}(E)$ is known, all physical quantities can be calculated by averaging first over the trajectories, and then over the energy. Let us test the theory at the strongest value of the interaction, at the apex of the new Coulomb diamond: $v = 1$ and $v_g = -1/2$. The orbits are quite simple for this case (see Fig. 3). The velocity is constant for $|x + 1/2| < 1/2$ and the trajectory is exactly half an ellipse for $|x + 1/2| > 1/2$. The averages of η_i and S on this trajectories lead to the following expressions for the probability

$$\mathcal{P}(E) = \mathcal{N}(1 + \pi\sqrt{2E})e^{-6E}/\sqrt{E}\,. \quad (10)$$

The current at the apex can be obtained by integrating expression (3) with the distribution (10). We find that $R_T I(v = 1, v_g = -1/2)/V = 1/(6 + 2\sqrt{3\pi}) \approx 0.0837$. With the same technique one can calculate the rms of x: $\sqrt{\langle (x - \bar{x})^2\rangle} = (40 + 3\sqrt{6}\,\pi^{3/2})^{1/2}/(96 + 8\sqrt{6}\,\pi^{3/2})^{1/2} \approx 0.628$.

The method can be applied to describe the transition from the blocked to the conducting state at finite v. In order to keep the calculation simple we consider $v \gg 1$. For $v_g = -v/2$ the minimum of the potential is at $x = 0$. The potential is harmonic for $x < 0$ with oscillation period 2π and harmonic for $x > 0$ with period $2\pi(1 - 1/v)^{-1/2}$. The oscillations will thus be more elongated inside the conducting regions (see Fig. 3). The calculation at leading order in $1/v$ gives the distribution: $\mathcal{P}(E) = \mathcal{N}[1 - 3\pi\sqrt{E}/(8v\sqrt{2}(1 - 1/v)^{1/2})]^{4(1-1/v)v}$. With this distribution we find that the current jumps at $v_g = -v/2$ (and symmetrically at $v_g = -v/2 - 1$) with $R_T I(v, v_g = -v/2^+)/V = (E_E/eV)\,8/(3\pi^2)[1 - 1/2v - 1/4v^2 + o(1/v^3)]$. For arbitrary values of v_g and v we found the analytical expressions for α and β and they have been used to obtain the current by numer-

ical integration. To check these results we have performed a Monte Carlo simulation of the model (see for instance Refs. [10, 15]). Fig. 4 shows the comparison for $v_g = -1/2$ and v varied between 0 and 8, and for fixed $v = 1.5$ and v_g varied between the blocked region to the degeneracy point (inset). We considered values Γ_o ranging from 10^{-2} to 10. Surprisingly, the agreement between the analytical and the numerical calculations is very good also for $\Gamma_o \ll 1$. Apparently the current depends very weakly on Γ_o (apart a trivial linear scaling).

Concerning the v_g dependence of the current (inset of Fig. 4) compare the exact result to the weak coupling result of Ref. [12] extrapolated to strong coupling (dashed line) or to the expression (3) taken at $x = x_m$ (long dashed line). For $v_g > -v/2$ the current flows through the device inducing a fluctuation of the position. The observed current is then the average of Eq. (3) over the values of x visited by the island. This average increases the current near the threshold, producing the discontinuity, and reduces it near the degeneracy point. Also for the rms of the position the analytical estimate given above agrees with the numerical simulation: for Γ_o varying in the same range of Fig. 4 we find that $\sqrt{\langle x - \bar{x} \rangle}$ ranges between 0.59 and 0.64, that compares well with the analytical result 0.628. The good agreement of the analytical and Monte Carlo results indicate that the analytical picture is accurate. It thus provide a simple and faithful description of device dynamics.

The presence of the mechanical bistability can be experimentally probed for $v < 1$ by modulating the gate voltage around -1/2: $v_g = -1/2 + v_g^o \sin(\omega t)$. According to the picture given before if $v_g^o < (1 - v)/2$, no current should flow, since the island remains in the same stable or meta-stable position all the time: v_g varies inside the dashed diamond of Fig. 2. For $v_g^o > (1 - v)/2$ the island is instead always released from the metastable state, and it is free to oscillate between the two positions $x = -1$ and $x = 0$. This implies that some current can flow through the device. The resulting DC current as a function of v_g^o is thus discontinuous at $v_g^o = (1 - v)/2$. In order to verify this idea quantitatively we resort to a Monte Carlo simulation for this non stationary situation. Results are shown in Fig. 5 for $v = 1/2$ and $\omega/\omega_o = 0.1$. For $v_g^o \gg (1 - v)/2 = 1/4$ we find that the current is one electron per cycle, regardless of the value of Γ_o. The value of the discontinuity depends instead strongly on Γ_o. For $\Gamma_o \gg 1$ many electrons can flow during the swing of the oscillator between the two stable solutions. In the opposite limit of $\Gamma_o \ll 1$, the discontinuity is strongly reduced. Nevertheless also in this case the nanomechanical nature of the current can be probed by studying the DC current as a function of the external frequency ω/ω_o. The inset shows the frequency dependence of the current at the threshold ($v_g^o = 1.05/4$) for large and small Γ_o. In both cases dips are present when $\omega/\omega_o = 0.5$, 1 or 2, indicating the resonant response of the mechanical degree of freedom.

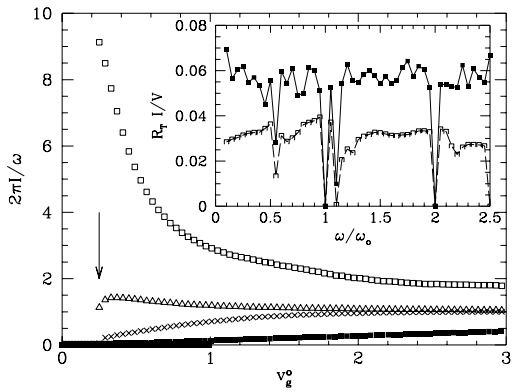

FIG. 5: DC current response to an oscillating gate voltage $v_g = -1/2 + v_g^o \sin(\omega t)$ as a function of v_g^o. $v = 1/2$, $\omega/\omega_o = .1$, (same symbols of Fig. 5) The arrow indicates the threshold to the conducting region. Inset: Frequency dependence of the DC current for $v_g^o = 1.05$ the threshold value. Structures at $\omega/\omega_o = 0.5$, 1 and 2 are clearly visible.

In conclusion we have shown that the coupling to a mechanical degree of freedom can lead to a current suppression at the degeneracy point. A bistability appears for $eV < E_E$ and we have shown how this can be detected by using an AC gate voltage. We also presented an analytic theory that allows to calculate with quantitative accuracy the current in the whole conducting region ($eV > E_E$). A gap at the degeneracy point has been already observed experimentally in different nanomechanical devices [4, 18]. The miniaturization of the devices will allow to increase further the value of E_E. Our predictions can be useful to test if the observed phenomena are really related to nanomechanical effects.

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